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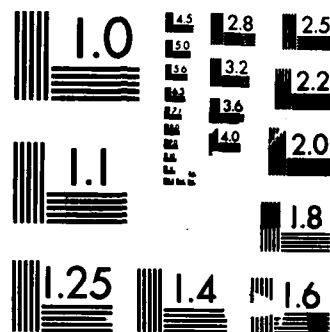
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# Thermal Expansion of Composites with Spherical and Cylindrical Inclusions

P.G. KLEMENS

*Composite Materials Branch  
Material Science and Technology Division*

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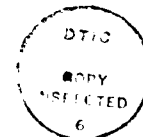
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## **THERMAL EXPANSION OF COMPOSITES WITH SPHERICAL AND CYLINDRICAL INCLUSIONS**

### **I. INTRODUCTION**

A composite which has inclusions of different thermal expansivity in a matrix will develop internal stresses as the temperature is changed. The overall coefficient of thermal expansion will therefore differ from the simple volume average.

Previous treatments by Eshelby<sup>(1)</sup>, by Wakashima et al.<sup>(2)</sup> and by Kerner<sup>(3)</sup> used the stress balance at the interface to find the strain field in terms of the misfit between inclusion and matrix, and are confined to linear elasticity. The present treatment derives these relations by minimizing the total strain energy. It uses an effective medium approximation, i.e. it replaced the properties of the matrix by those of the material as a whole, but assumes that the short-range shear strain about each inclusion depends only on the shear modulus of the matrix. Also it expresses the result in terms of bulk moduli and shear moduli, since this is convenient when separating the strain field into dilation and shear components. This formulation facilitates the extension of the theory into the plastic regime. The treatment is confined to inclusions which are spherical or randomly oriented long cylinders.

## II. ELASTIC FIELD AROUND A SPHERICAL INCLUSION

Consider a spherical hole of radius  $R$  cut out of the matrix, with a spherical inclusion of radius  $R + \Delta R_2$  forced into the hole (if  $\Delta R_2 > 0$ ), or placed into the hole with the surrounding matrix forced to join the inclusion (if  $\Delta R_2 < 0$ ). The hole expands or contracts to a radius  $R + \Delta R$ .

A point in the matrix, of distance  $r$  from the center, undergoes a displacement  $u(r)$ , which must be of the form

$$u(r) = Ar + B/r^2 \quad (1)$$

and in particular

$$u(R) = \Delta R \quad (2)$$

The spherical inclusion changes its radius by  $\Delta R_2 - \Delta R$ ; it changes its volume, and there is an associated strain energy. If the fractional volume of inclusions is  $c$ , the energy of compression of the inclusions, per unit volume of material, is

$$E_{\text{incl}} = \frac{9}{2} c K_I (\Delta R_2 - \Delta R)^2 / R^2 \quad (3)$$

where  $K_I$  is the bulk modulus of the inclusion.

The term  $Ar$  in (1) corresponds to a uniform expansion of the matrix; the strain energy per unit volume of material is

$$E_{\text{exp}} = \frac{1}{2} K_M 9A^2 (1-c) \quad (4)$$

where  $K_M$  is the bulk modulus of the matrix.

In addition, the matrix suffers shear because of the non-dilatational displacement  $u = B/r^2$ . The principal strains, which are along the radial direction and any two mutually perpendicular directions normal to it are,

$$e_{rr} = \partial u / \partial r = -2B/r^3 \quad (5a)$$

$$e_{yy} = e_{zz} = u/r = B/r^3 \quad (5b)$$

The shear strain energy density becomes

$$\begin{aligned} W_{sh} &= \frac{1}{2} \sum 2\mu e_{ij}^2 + \frac{1}{2} \lambda \Delta^2 \\ &= \mu B^2 r^{-6} (4+1+1) = 6 \mu B^2 / r^6 \end{aligned} \quad (6)$$

since the dilation  $\Delta = e_{rr} + e_{\theta\theta} + e_{zz}$  vanishes. Here  $\mu$  is the shear modulus of the matrix,  $\lambda$  is the other Lamé modulus. Integrating over the volume of the matrix, i.e. from  $r = R$  to infinity

$$\begin{aligned} E_{shear} &= \int_R^\infty 4\pi r^2 W_{sh}(r) dr = (4\pi/3) 6\mu B^2 / R^3 \\ &= (4\pi R^3/3) 6\mu (B/R^3)^2 \end{aligned} \quad (7)$$

Expressing this per unit volume of material, where  $c$  can be equated to  $4\pi R^3/3$ ,

$$E_{shear} = 6\mu c (B/R^3)^2 \quad (8)$$

The total strain energy per unit volume of material thus becomes

$$E = (9/2) c K_I (\Delta R_2 - \Delta R)^2 / R^2 + (9/2)(1-c) K_M A^2 + 6\mu c (B/R^3)^2 \quad (9)$$

where

$$\Delta R = R (A + B/R^3) \quad (10)$$

Here  $K_I$ ,  $K_M$  are the bulk moduli of the inclusion and the matrix respectively,  $\mu$  is the shear modulus of the matrix,  $c$  is the volume fraction occupied by inclusions,  $A$  and  $B/R^3$  are linear strain parameters and  $\Delta R_2$  is the linear misfit between inclusion and matrix.

One can define two strain parameters

$$\beta = B/R^3 \quad (11)$$

and

$$\gamma = \Delta R_2 / R \quad (12)$$

Now the condition of elastic stability is that the total strain energy  $F$

should be a minimum; two stability conditions must be satisfied

$$\partial E / \partial A = 0 \quad (13a)$$

and

$$\partial E / \partial \beta = 0 \quad (13b)$$

Since  $(\Delta R_2 - \Delta R) / R = \gamma - A - \beta$ , equation (13a) yields

$$9c K_I (\gamma - A - \beta) = 9(1-c) K_M A \quad (14a)$$

and (13b) yields

$$9c K_I (\gamma - A - \beta) = 12 \mu c \beta \quad (14b)$$

Eliminating the left-hand side of both equations

$$A = \frac{c}{1-c} \beta \frac{4\mu}{3K_M} \quad (15)$$

Eliminating A from (14a and b)

$$\beta = \gamma \left[ 1 + \frac{4\mu}{3K_I} + \frac{4\mu c}{3K_M(1-c)} \right]^{-1} \quad (16)$$

and eliminating  $\beta$  from (15) and (16)

$$A = \gamma \frac{c}{1-c} \frac{4\mu}{3K_M} \left[ 1 + \frac{4\mu}{3K_I} + \frac{4\mu c}{3K_M(1-c)} \right]^{-1} \quad (17)$$

### III. APPLICATION TO THERMAL EXPANSION

The volume expansion comes from two sources: the A-field is a uniform expansion of the matrix and the included cavities, while the  $\beta$ -field represents an additional expansion of the included cavities. This latter field is non-dilational, and transmits that expansion to the outer boundaries, since  $\delta V_B = 4\pi r^2 B / r^2$  is independent of  $r$ . Therefore

$$\delta V / V = 3A + 3c\beta \quad (18)$$

Now let the matrix have a volumetric thermal expansion coefficient  $d\Delta_M/dT$ , and the inclusions a coefficient  $d\Delta_I/dT$ , then the overall coefficient of thermal expansion is

$$\begin{aligned} d\Delta/dT &= d\Delta_M/dT + \frac{d}{dT} (\delta V/V) \\ &= d\Delta_M/dT + \frac{d}{dT} (3A + 3c\beta) \end{aligned} \quad (19)$$

where  $A$  and  $\beta$  can be expressed in terms of  $\gamma$  through (16) and (17).

Now for an isolated inclusion

$$3 d\gamma/dT = d\Delta_I/dT - d\Delta_M/dT \quad (20)$$

but if  $c$  is not small,  $d\Delta_M/dT$  should be replaced by the actual expansion of the composite, which is  $d\Delta/dT$ . This takes account, to some degree, the interaction between inclusions; in addition,  $K_M$  should be replaced by the average bulk modulus of the material

$$\bar{K}_M = (1-c) K_M + c K_I \quad (21)$$

On the other hand, the shear field  $B/r^3$  is short-range, and if the inclusions do not touch too frequently,  $\mu$  should be taken as the shear modulus of the matrix. Thus replacing (20) by

$$3d\gamma/dT = d\Delta_I/dT - d\Delta/dT \quad (22)$$

equation (19) becomes, using (16) and (17)

$$d\Delta/dT = d\Delta_M/dT + 3c (d\gamma/dT) F(\mu) \quad (23)$$

Using (22), one finally obtains

$$(1+cF) d\Delta/dT = d\Delta_M/dT + cF d\Delta_I/dT \quad (24)$$

where

$$F(\mu) = \frac{1 + 4\mu/3(1-c)\bar{K}_M}{1 + 4\mu/3K_I + 4c\mu/3(1-c)\bar{K}_M} \quad (25)$$

is a function of  $\mu$ .

To obtain the net dilation over a finite temperature interval, one has to integrate (24) over temperature, i.e.

$$\Delta(T) = \int_{T_0}^T \frac{d\Delta(T)}{dT} dT \quad (26)$$

It is relatively straight forward to take account of temperature dependences of  $d\Delta_M/dT$  and  $d\Delta_I/dT$ . Similarly  $K_I$  and  $\bar{K}_M$  can be regarded as temperature dependent, although usually only weakly so.

The shear modulus  $\mu$  is defined by

$$2\mu = d\sigma_{ij}/d\epsilon_{ij} \quad i \neq j \quad (27)$$

where the stress and strain tensors  $\sigma$  and  $\epsilon$  are expressed in the contracted notation. Now  $\mu$  is not only a function of temperature, but in the plastic regime also a function of prior shear strain. Since the shear strain is a function of radial distance  $r$  (see equations 5 and 6),  $\mu$  is also a function of  $r$ , and therefore the present treatment is strictly speaking invalid once the plastic regime is reached.

#### IV. EFFECT OF PLASTICITY

Although  $\mu$ , which depends on prior shear strain, is different at different points of the matrix, since the shear strain is a function of position, one notes that most of the shear strain energy of (7) resides in the immediate vicinity of the inclusion, where the shear strain is a maximum, and is given in magnitude by  $\beta=B/R^3$ . To a good approximation one may thus regard  $\mu$  of equation (24) to be only a function of  $\beta$  and  $T$ .

In the absence of plasticity, from (16) and (22)

$$d\beta = f(\mu)^{-1} d\gamma \quad (28)$$

where

$$f(\mu) = 1 + \frac{4}{3} \left( \frac{\mu}{K_I} + \frac{c\mu}{(1-c)K_M} \right) \quad (29)$$

and where

$$d\gamma = (1/3) (d\Delta_I/dT - d\Delta/dT) dT \quad (30)$$

In calculating  $\Delta(T)$  from (24) one must check that  $\beta = \int d\beta(T) dT$  is small enough so that plastic effects do not occur. Once  $\beta$  and  $T$  are large enough so that plasticity is significant,  $\mu(\beta, T)$  must be determined from the appropriate model of plasticity. As  $T$  is increased by a finite step  $dT$ , the incremental expansion  $d\Delta$  must be determined from (24), and the increment in shear strain then determined from

$$d\beta = (1/3) (d\Delta_I - d\Delta) / f(\mu) \quad (31)$$

The new value of  $\Delta$ , namely  $\Delta + d\Delta$ , and the new value of  $\beta$ , namely  $\beta + d\beta$ , are then used to determine a new value of  $\mu$ , and this value is used in (24) and (31) for the next temperature increment. This procedure seems suited for a programmable computer.

## V. ELASTIC FIELD AROUND AN INFINITE CYLINDER

The displacement field  $u(r, \theta, z)$  about an infinite cylinder obeys the elastic equations

$$\frac{\partial}{\partial r} \left( \frac{\partial u}{\partial r} + \frac{u}{r} \right) = 0, \quad \partial^2 u / \partial z^2 = 0 \quad (32)$$

and the solution is of the form

$$u_r = (Ar + B/r), \quad u_z = e_0 z \quad (33)$$

The principal strains are

$$e_{zz} = e_0 \quad (34a)$$

$$e_{rr} = \partial u / \partial r = A - B/r^2 \quad (34b)$$

$$e_{\theta\theta} = u/r = A + B/r^2 \quad (34c)$$

and the dilation is

$$\Delta = 2A + e_0 \quad (35)$$

The principal stresses are

$$\sigma_{rr} = 2\mu(A - B/r^2) + \lambda\Delta \quad (36a)$$

$$\sigma_{\theta\theta} = 2\mu(A + B/r^2) + \lambda\Delta \quad (36b)$$

$$\sigma_{zz} = 2\mu e_0 + \lambda\Delta \quad (36c)$$

where  $\lambda$ ,  $\mu$  are the Lamé moduli. The strain energy density is given by

$$\begin{aligned} W(r) &= 1/2 \sigma_{rr} e_{rr} + 1/2 \sigma_{\theta\theta} e_{\theta\theta} + 1/2 \sigma_{zz} e_{zz} \\ &= \mu(A - B/r^2)^2 + \mu(A + B/r^2)^2 + \mu e_0^2 + 1/2 \lambda \Delta^2 \\ &= 2\mu A^2 + 2\mu B^2/r^4 + \mu e_0^2 + 1/2 \lambda (2A + e_0)^2 \end{aligned} \quad (37)$$

Now consider a random assembly of cylinders, filling a fraction  $c$  of the entire volume. Let the length of each cylinder experience the same fractional increase as any random line in the matrix, so that  $e_0 = A$ . The strain energy of the matrix is obtained by integrating the B-field energy density from  $r=R$  to  $r=\infty$ , and adding to it the dilatational energy of the A-field, which is a uniform expansion. Thus

$$\begin{aligned} E_B &= 2\mu B^2 \int_R^\infty 2\pi r r^{-4} dr = 2\pi\mu B^2/R^2 \\ &= 2\mu(B^2/R^4) (\pi R^2) \end{aligned} \quad (38)$$

Note that  $\pi R^2$  is the volume per unit length of the inclusions, so that, per unit volume,  $E_B = 2\mu(B^2/R^4)c$ . For the shear modulus of the matrix we take that of the matrix material, assuming that since most of the strain energy is in the immediate vicinity of the inclusion, the significant material is that of the matrix. Now  $K_M = (\lambda + 2\mu/3)$  is the bulk modulus of the matrix. The dilational energy can thus also be written as  $1/2 K_M (3A)^2$ , and since the matrix occupies a fractional volume  $(1-c)$  only, this energy must be multiplied by that factor  $(1-c)$ . Furthermore,  $K_M$  should really be the volume average of the matrix and the inclusions, so that, per unit volume

$$E_A = 1/2 (1-c)(3A)^2 [(1-c) K_M + c K_I] \quad (39)$$

where  $K_I$  is the bulk modulus of the inclusion material. The strain energy of the matrix material, per unit volume becomes thus

$$E_M = E_A + E_B = 1/2 (1-c) K_M' (3A)^2 + 2c\mu_M B^2/R^4 \quad (40)$$

where  $K_M'$  is the volume-averaged bulk modulus.

Now the strain field arises, in the first place, because each cylindrical inclusion, when unstrained, occupies a different volume than the cylindrical cavity of the unstrained matrix. Let the original radius of the cylindrical inclusion be  $R + \Delta R_2$ ; it sits in a matrix cavity of radius  $R + \Delta R$ , where

$$\Delta R = \Delta R_1 + B/R \quad (41)$$

Let us also assume that originally there is a longitudinal strain between the unstrained matrix and the inclusion, of magnitude

$$e_2 = \Delta R_2/R \quad (42)$$

Thus the original length of the inclusion

$$1 + e_2 = 1 + \Delta R_2/R \quad (42')$$

is changed to  $1+A$ . The inclusion thus has the following principal strains:

$$\Delta R_2/R - \Delta R/R \quad (2 \text{ transverse components})$$

$$\Delta R_2/R - A \quad (1 \text{ longitudinal component})$$

and a net dilation

$$\Delta_I = 3\Delta R_2/R - 2\Delta R/R - A \quad (43a)$$

and in view of (41)

$$\Delta_I = 3\Delta R_2/R - 3A - 2B/R^2 \quad (43b)$$

This strain field, uniform within the inclusion, can be resolved into a dilation  $\Delta$  of (43b), and three principal strains of zero dilation, of magnitude

$$-2B/R^2, B/R^2 \text{ and } B/R^2$$

so that, per unit volume of material, the strain energy within the inclusions becomes

$$E_I = 1/2 c K_I \Delta^2 + 6c\mu_I B^2/R^4 \quad (44)$$

while the total strain energy per unit volume becomes

$$E = E_M + E_I = (9/2) K_M^I (1-c) A^2 + 2c\mu_M B^2 + 6c\mu_I B^2 + (9/2)c K_I (\gamma - A - 2\beta/3)^2 \quad (45)$$

where  $\beta = B/R^2$  and  $\gamma = \Delta R_2/R$ .

The conditions of stability are that

$$\partial E / \partial A = 0 \text{ and } \partial E / \partial \beta = 0 \quad (46)$$

which becomes

$$9K_M^I (1-c)A = 9K_I c (\gamma - A - 2\beta/3) \quad (47a)$$

$$4(\mu_M + 3\mu_I)c\beta = 6K_I c (\gamma - A - 2\beta/3) \quad (47b)$$

Eliminating  $\gamma$  we obtain

$$A = \frac{2}{3} \frac{c}{1-c} (\mu_M + 3\mu_I) \beta / K_M' \quad (48)$$

Substituting (48) into (47b) we obtain

$$\beta = \frac{3}{2} \gamma \left[ 1 + \frac{\mu_M + 3\mu_I}{K_I} + \frac{c}{1-c} \frac{\mu_M + 3\mu_I}{K_M'} \right]^{-1} \quad (49)$$

Finally, from (48) and (49)

$$\begin{aligned} A &= \frac{c}{1-c} \gamma \left[ \frac{\mu_M + 3\mu_I}{K_M'} \right] \left[ 1 + \frac{\mu_M + 3\mu_I}{K_I} + \frac{c}{1-c} \frac{\mu_M + 3\mu_I}{K_M'} \right]^{-1} \\ &= \frac{c}{1-c} \gamma \left[ \frac{K_M'}{\mu_M + 3\mu_I} + (K_M'/K_I) + c/(1-c) \right]^{-1} \end{aligned} \quad (50)$$

Thus, given  $\gamma$ , one can find  $A$  and  $\beta$ .

## VI. VOLUME CHANGE AND THERMAL EXPANSION

The strain field just discussed causes a net dilation

$$\Delta = 3A + 2c\beta \quad (51)$$

The first term is a uniform expansion of the matrix and of the cylindrical cavities which hold the inclusions; the second term is the additional expansion which does not dilate the matrix but transmits the expansion of the cylinders to the outside surface. This can be expressed in terms of the misfit parameters  $\gamma$  through (49) and (50). Writing

$$f(\mu_M, \mu_I) = 1 + \frac{\mu_M + 3\mu_I}{K_I} + \frac{c}{1-c} \frac{\mu_M + 3\mu_I}{K_M'} \quad (52)$$

equation (51) becomes

$$\Delta = 3c\gamma \left[ 1 + \frac{\mu_M + 3\mu_I}{(1-c)K_M'} \right] f^{-1} \quad (53)$$

In the special case when  $K_I = K_M$  and hence  $K_I = K_M'$ , (53) becomes simply  $\Delta = 3c\gamma$ , so that the excess volume of the cylindrical inclusions, weighted by  $c$ , becomes simply the net increase in volume: the compression of the inclusions

by the matrix is compensated by the expansion of the matrix. In general, however, the expansion is larger than  $3c\gamma$  if  $K_I > K_M$ , and vice versa.

Suppose now that the misfit parameter  $\gamma$  is caused by a difference in thermal expansivity of matrix and inclusions, so that as in (20)

$$3d\gamma/dT = d\Delta_I/dT - d\Delta_M/dT \quad (54)$$

Writing

$$F(\mu_M, \mu_I) = (1 + \frac{\mu_M + 3\mu_I}{(1-c)K_M})/f \quad (55)$$

where  $f$  is given by (52), adding the thermal expansion of the matrix to that due to the misfit (equation 53) we obtain

$$d\Delta/dT = d\Delta_M/dT + 3cF d\gamma/dT \quad (56)$$

With the same self-consistency approximation as was made for spherical inclusions we replace  $d\Delta_M/dT$  in (54) -but not in the first term of (56) -by  $d\Delta/dT$ , and obtain, as in (24), that

$$(1+cF) d\Delta/dT = d\Delta_M/dT + cF d\Delta_I/dT \quad (57)$$

the only difference being that  $F$ , previously defined by (25), is now given by (55).

When accounting for plasticity, we must remember that  $F$  is now a function of two shear moduli,  $\mu_M$  and  $\mu_I$ . We must still make the approximation, not as well justified for cylinders as for spheres, that  $\mu_M$  is just a function of  $\beta$  and  $T$ , since the shear strain energy in the matrix resides mainly just near the interface. In the inclusions, however, the shear strain is uniform, so that no approximation is incurred when treating  $\mu_I$  as just a function of  $\beta$  and  $T$ . One can then proceed analogously to the case of spherical inclusions, obtaining  $\Delta(T)$  by numerical integration.

## VII. CONCLUSION

By minimizing the strain energy and making use of the fact that the strain field is composed of a uniform dilation of the matrix and a short-range shear strain field, it is possible to obtain closed expressions for the overall thermal expansion in the case of spherical inclusions and of randomly oriented long cylindrical inclusions. A procedure was obtained for extending the results to the case of plastic flow of the matrix about the inclusion, if plastic behavior can be expressed as an effective shear modulus as function of temperature and shear strain.

Expressions were also obtained for the dilation of the matrix in terms of the misfit between matrix and inclusion, and thus also in terms of the overall expansion. These could be used to test the model by comparing dilatometry with changes of the lattice spacing of the matrix. These results could also be used in related problems, such as comparing the swelling due to radiation damage to the corresponding changes of the lattice spacing of a material.

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